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Reactive Transport Modeling for Desalination Systems

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The increasing interest in the use of membrane systems to desalinate inland brackish water, agricultural drainage water, or industrially produced wastewater demands an improved understanding of the effect of variable feedwater compositions on the systems' performance. The interaction among water flow, solute transport, and geochemical reactions impacts permeate fluxes and their evolution in time. There exists an opportunity to bring to bear reactive transport modeling on desalination systems. For this purpose, we develop a reactive transport model that simulates these coupled processes for the prediction of permeate fluxes. The geochemical component includes multicomponent aqueous equilibrium, the Pitzer ion interaction formalism, and mineral precipitation. Flow and transport are solved with an approach that allows for efficient simulation of large domains while still capturing concentration polarization. We use the model to simulate reverse osmosis in benchtop crossflow experiments and membrane modules for a range of feed flow rates and compositions, under fouling and non-fouling conditions. We show that solutions with the same or similar total dissolved solids but different compositions may have a different geochemical evolution during desalination. In membrane systems, this results in different permeate fluxes. This result shows the need to consider these coupled processes together and demonstrates the value of reactive transport modeling in this application.